Analysis of Transient Quantum Transport in Nanoscale Devices Using Density Matrix Methods

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***Abstract*—The study of quantum transport in open devices based on density matrix methods such as the Wigner transport equation provides many benefits, most importantly the ability to model time-resolved phenomena such as intrinsic oscillations in resonant tunneling diodes or amplifier behavior of gate-all-around FETs. Considering that the transport equations can be solved using different basis sets, discretization schemes and boundary conditions, a variety of different approaches emerges. Meanwhile, the optimal method may change based on the simulation requirements. Therefore, an overview of the different techniques when applied to open devices in engineering applications is given here with a focus laid on the comparison of the phase space methods to those solved in real space.**

***Index Terms*—transient, quantum transport, density matrix, wigner, von-neumann, tight-binding, quantum-liouville, discontinuous galerkin.**

I. Introduction

As semiconductor devices continue to scale, the growing complexity of atomistic effects also leads to increasingly demanding requirements for the simulation models. These requirements include but are not limited to the appropriate treatment of open contacts and allowing for the inclusion of multiband models, in addition to taking into account scattering effects, all while maintaining computational efficiency. The latter point is important in particular for the time-resolved case, where non-equilibrium Greens function (NEGF) methods are still plagued with an extreme computational burden as of now [1]. The application of density matrix based methods, however, is especially well-suited for this case, with several different approaches to chose from. These can mainly be divided into phase space methods such as the Wigner Transport Equation (WTE) [2] and quantum-Liouville-type equation (QLTE) (Fig. 1a) [3], and real space methods which solve either a Heisenberg equation or the von-Neumann equation (VNE) for the density matrix in real space (Fig. 1b) [4]. While the WTE is arguably the most well known and historically most used of the methods due to its similarity to the Boltzmann equation and ease of including inflow boundary conditions, the real space methods, especially in conjunction with a tight-binding description can offer several advantages. Inflow boundary conditions can still be included in this case with the introduction of a local Fourier transform at the contacts [5] (see Fig. 2).

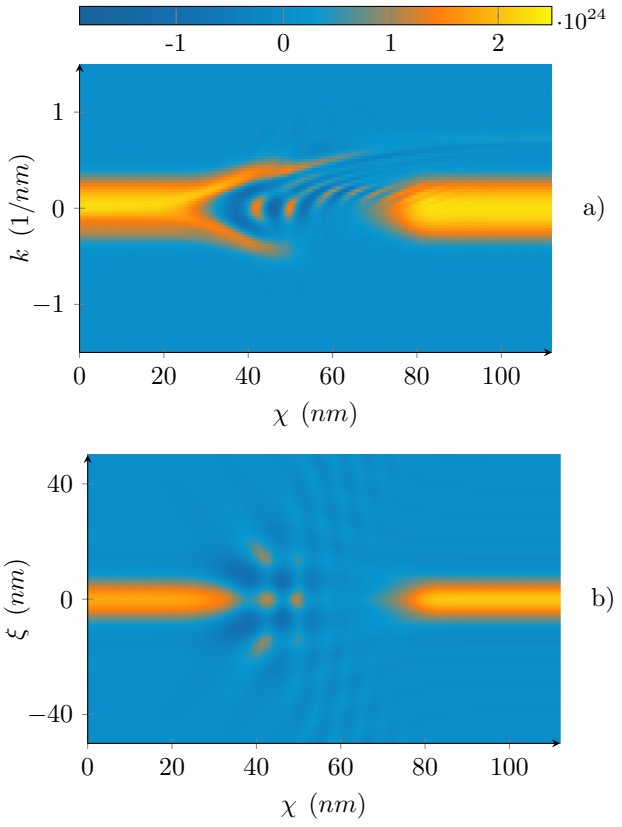

Fig. 1. The real parts of the Wigner function (a) and density matrix (b) are shown for the same bias voltage applied to an exemplary RTD. The two functions are analytically linked by a Fourier transform along the ξ-coordinate if the same Hamiltonian is used.

Therefore, the benefits and drawbacks of each method, along with the appropriate discretization methods are presented in the following sections, accompanied by results when applied to the exemplary devices of the resonant tunneling diode (RTD) (Fig. 3 and Fig. 4), the gate-all-around FET (GAAFET) shown in Fig. 5, and a squeezed channel GAAFET (Fig. 6 and Fig. 7). Even though scattering is neglected here, relaxation time approaches can easily be included [3] with all approaches.

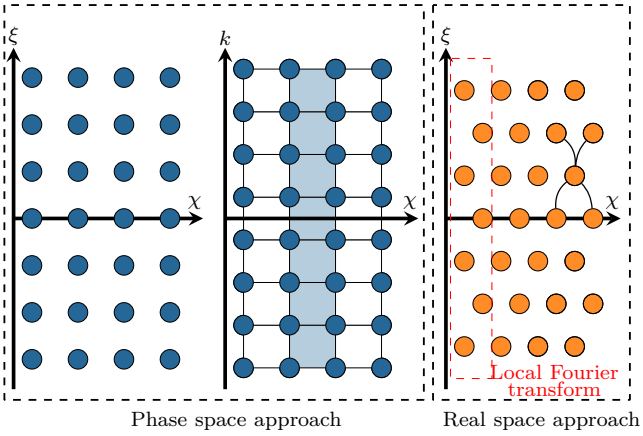

Fig. 2. The derivation of the Wigner function is schematically shown on the left hand side, where usually a uniform grid in real space is assumed, before applying the Fourier transform along the ξ-direction. The tight-binding real space formulation is schematically shown on the right side with the density matrix elements defined on the same lattice sites as the Hamiltonian with the curved lines representing coupling terms between density matrix elements. The Fourier transform is only needed at the contacts as is indicated by the dashed red rectangle.

II. Phase Space Based Methods

The use of phase space methods naturally follows from the need to distinguish between in- and outgoing waves when setting up the inflow boundary conditions accounting for the nature of open devices [6]. The WTE governing the temporal evolution of the Wigner function is arguably the most widely used of the phase space methods, with a wealth of research conducted [2] and applications in both electron and phonon transport modeling [7], as well as electron-phonon scattering [8]. Results obtained by the WTE agree well with those obtained through reference results, in particular if a complex absorbing potential (CAP) is added [9] to minimize reflections at the edges of the finite computational domain in k-direction. The same applies to the closely related QLTE which is obtained by replacing the analytical Fourier transform when deriving the Wigner function with a basis expansion onto e.g. plane waves or eigenfunctions of the diffusion operator, thereby further improving the computational efficiency when reducing the number of basis vectors [3]. However, as is demonstrated in Fig. 2, the necessity of the phase space transform along the ξ axis by either a Fourier transform or the basis expansion also limits the possibilities of including non-uniform grid and thus, inclusion of heterostructures with varying lattice distances.

With relatively few exceptions, e.g. [10], most work on density matrix electron transport is based a continuum Hamiltonian in the effective mass approximation $\hat{\mathcal{H}} = -\frac{\nabla^2}{2m^*} + V(\boldsymbol{r})$, e.g. [3], [5], [6]. This can pose several disadvantages, for example when applying the coupled mode space approximation [11], [12] to the squeezed channel GAAFET shown in Fig. 6. As the coupling terms depend on the explicit derivative of the modal wave functions, they can be ill-defined at the interface and difficult to capture from a numerical standpoint [12].

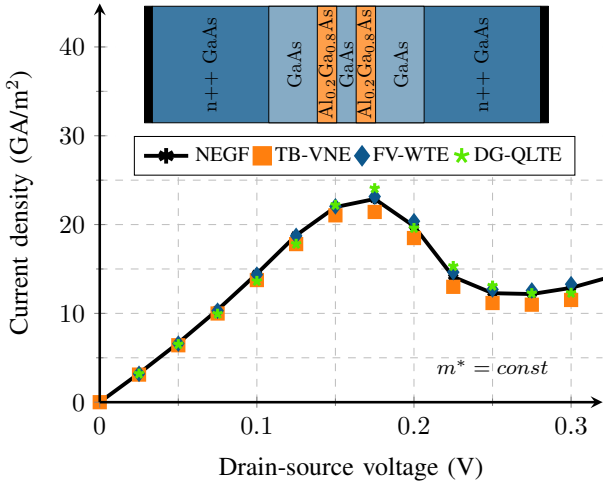

Fig. 3. Reference current densities from the NEGF method are compared to results obtained by a tight-binding (central difference) von-Neumann equation (TB-VNE), finite volume WTE (FV-WTE) and discontinuous Galerkin method QLTE (DG-QLTE). All agree well with each other for the flatband simulation of a GaAs/AlGaAs RTD with an assumed constant effective mass.

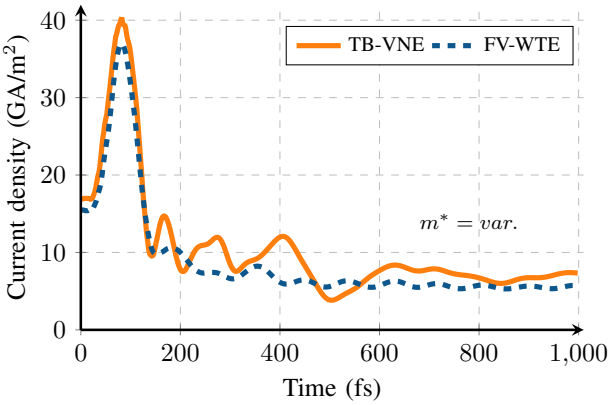

Fig. 4. The time-resolved current densities obtained by the TB-VNE and FV-QLTE are shown for a change in applied drain-source voltage from 0.15 V to 0.25 V at $t = 0$ fs for the same RTD as shown in Fig. 3, albeit with the inclusion of a spatially varying effective mass in the barrier regions.

A. Discretization methods

Common discretization methods of the WTE and QLTE consist of finite difference upwind schemes (UDS), Monte Carlo sampling (MC) and finite volume methods (FV). Additionally, efficient finite element methods like the discontinuous Galerkin method (DG) have also been investigated [13]. Further analyzing the deterministic methods and excluding upwind schemes due to inherent numerical difficulties [14], the strengths of the FV method lie in both the wealth of research conducted and numerical robustness [3], [14]. By deriving the discretization pattern from a phase-space exponential operator, a norm-conserving formulation is achieved that can easily be adapted to include higher order derivatives or a position-dependent effective mass [14]. In comparison, the DG method can offer significant reductions in computation time for the

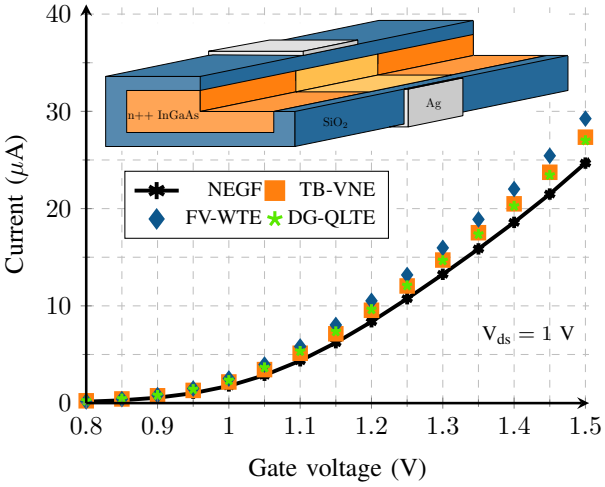

Fig. 5. For multigate devices such as GAAFETs the previously mentioned approaches can be combined with the mode-space approximation [11]. The self-consistent results of all methods agree well with each other and reference results obtained by a coupled mode space NEGF method.

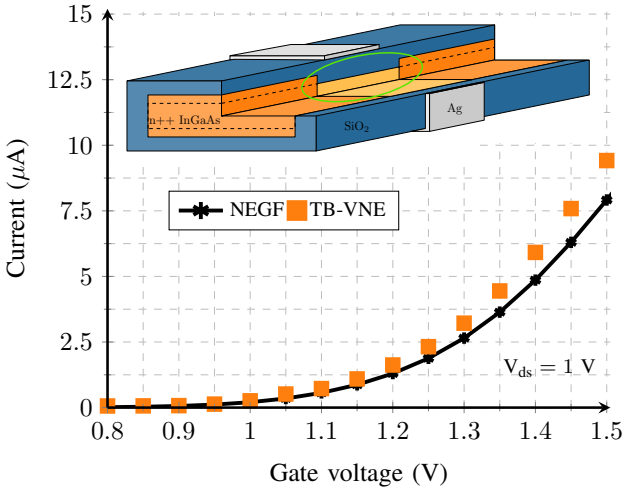

Fig. 6. If the channel dimensions of the GAAFET are modulated, coupling between the modes is induced and the rapidly changing coupling terms are difficult to capture with continuum models [12]. The real space method based on the tight-binding VNE is better suited for these kinds of devices and the self-consistent drain-end current agrees well with reference results from the NEGF method. No solution using the WTE or QLTE based on a continuum Hamiltonian could be obtained.

transient case due to its explicit nature and high parallelization by utilizing the globally block-diagonal system matrix [13]. Still, the numerical flux requiring the use of limiters to obtain stability proves to be challenging.

However, all of the above discretization methods approach their limits when applying such continuum models onto devices just few atoms in dimension where a more atomistic description may be helpful [12]. Again, for the case of the squeezed channel GAAFET the coupling terms are sharply varying at the interface, which can be hard to capture numerically both in the Fourier transform and when integrating over the numerical cell (indicated by the blue shaded areas in Fig. 2) in the finite volume scheme.

III. Real space based methods

Even though the already mentioned discretization methods can also be applied to solving the VNE (e.g. finite difference scheme used in [5]), the real space formulation naturally lends itself to the use of atomistic models like tight-binding Hamiltonians [4]. When inserted into a Heisenberg equation of motion along with the density operator defined in terms of field operators, a density matrix formalism in second quantization is obtained:

$$-\imath\hbar\frac{d}{dt}\rho_{ls} = \sum_u \gamma_{ul}\rho_{us} - \sum_m \gamma_{ms}\rho_{lm} + (\epsilon_l - \epsilon_s)\rho_{ls}, \quad (1)$$

with the density matrix elements defined as the expectation values of pair operators $\rho_{ls} = \langle \hat{c}_l^\dagger \hat{c}_s \rangle$ and hopping and onsite terms γ and ϵ, respectively. Instead of a somewhat arbitrarily chosen computational grid as is used with the WTE, the density matrix elements are defined on the same lattice points as those of the tight-binding Hamiltonian, with a resulting discrete equation of motion similar to when a finite difference scheme is used. One of the main benefits is that problems regarding the non-unitary transforms in the conventional phase space approach are circumvented [6] and an atomistic description appropriate for nanoscale devices is retained, so that changes in device geometry (Fig. 6) and heterostructures with varying interatomic distances pose no problem [4]. The inflow boundary conditions can be included by using a local Fourier transform at the contacts [5] which is readily incorporated into the system matrix. Similar to the DG formulation mentioned earlier, explicit methods in the time domain can be used, where the high sparsity of the system matrix is an additional computational benefit. For the RTD shown in Fig. 3 the results agree well with those obtained by the phase space and NEGF methods, both for the case of a constant effective mass and if the spatial variation of the effective mass in the barriers is taken into account [4]. For the transient case depicted in Fig. 4 the current density obtained from the real space method shows some minor oscillations between 200 and 600 fs that are not seen with the FV WTE method, likely stemming either from the difference in inclusion of boundary conditions or from effects captured in the tight-binding Hamiltonian not present with the use of a continuum effective mass Hamiltonian. When applied to the squeezed channel GAAFET, the previously mentioned difficulties pertaining to the continuum Hamiltonian and discretization schemes are circumvented and discontinuities can easily be taken into account with resulting drain-end currents less than half of those from the non-squeezed GAAFET at the same gate voltages (Fig. 6). The results obtained by this method also agree with those obtained through a coupled mode-space NEGF method [12], however the density matrix formalism allows for further analysis of the time-resolved carrier transport as is demonstrated in Fig. 7 for the case of amplifier operation.

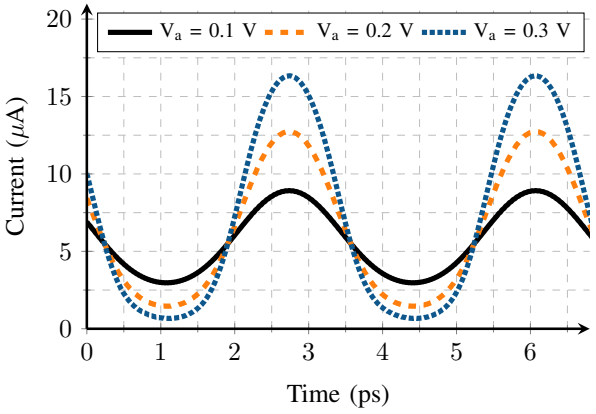

Fig. 7. The time-resolved drain-end current obtained from the TB-VNE is shown for the GAAFET from Fig. 6. The transistor is in AB operation with its operating point $V_{\text{op}} = 1.387$ V chosen by $V_{op} = V_{\text{threshold}} + 0.25$ V. A sinusoidal signal at $f = 300$ GHz is applied to the gate with three different amplitudes V_{a}. The resulting current can be further analyzed, e.g. regarding amplifier and mixing behavior.

IV. Conclusion

The WTE and QLTE provide an easy to implement and efficient model that is applicable to numerous devices and transport problems, and can be paired with both conventional (e.g. finite volume) and novel discretization methods. The QLTE formalism in particular is well suited for the combination with the FV and DG discretization schemes for numerous single- and multiband applications where the use of a continuum effective mass Hamiltonian is appropriate. However, if a more atomistic description is needed, the inclusion of a tight-binding Hamiltonian may be more suitable and the real-space method is the better option. With the inclusion of a local Fourier transform at the contacts, inflow boundary conditions can still be included in this case and results agree well with stationary and transient values from the phase space methods and stationary results from the NEGF method.

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